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Interactive Visual Least Absolutes Method: Comparison with the Least Squares and the Median Methods

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Ⓢ *Supporting Information*

ABSTRACT: A visual regression analysis using the least absolutes method (LAB) was developed, utilizing an interactive approach of visually minimizing the sum of the absolute deviations (SAB) using a bar graph in Excel; the results agree very well with those obtained from nonvisual LAB using a numerical Solver in Excel. These LAB results were compared with those from the popular least-squares method (LSQ), which minimizes the sum of the squares of the deviations (SSQ), and also with results from the median method (MED). LAB yielded similar results as LSQ for a data set with relatively smaller average deviations (<5%) as well as for data sets with relatively larger average deviations (>10%). However, for data sets with an outlier, the LAB method yielded significantly different results than LSQ. The LAB results, in all three cases, agree more closely with the results from MED of Theil and Siegel, which handles outliers better than the LSQ approach. The LAB approach (visual or numerical) is as simple and easy to implement in a spreadsheet as LSQ. The visual LAB approach may be practiced for analyzing data that requires regression in any college laboratory courses, especially when the data contain suspected outliers, because it is pedagogically more effective for visual learners than the numerical LAB with Solver.

KEYWORDS: *Demonstrations, First-Year Undergraduate, Computer-Based Learning, UV−Vis Spectroscopy*

■ BACKGROUND

Despite its weakness of not being robust or resistant, the least-squares method (LSQ) has been one of the most commonly practiced statistical methods for over a century. Numerous books (refs 1−5 to name a few) and articles have been published on the subject; this Journal alone has published over four dozen articles with the subject in the title, expounding the method and its applications (refs 6−10 to name a few among many). When all fields in both the natural and social sciences are combined, the number of publications is enormous. The popularity and dominance of LSQ is due largely to its effective handling of regression analysis. Its well-defined analytical solution for the regression parameters and variance analysis, guaranteeing minimum variance estimates of the parameters, has resulted in handy prepackaged formulas for scientific calculators and spreadsheet software programs for computers. The weakness of the LSQ arises from the assumption of normal distribution of errors in data, which also implies that the data contains enough number of measurements (n), preferable $n > 15$; in many instances, however, this is hardly the case, n being less than 10 in many lab experiments. Thus, LSQ is not statistically robust (meaning it is "insensitive to departure from assumptions surrounding an underlying probabilistic model"),[11] and it is not resistant (meaning it is "too sensitive to localized misbehavior in data").[12] Namely, it has the drawback of exaggerating the effects of data with larger deviations compared with data with smaller deviations. The problem becomes serious with data containing an outlier,[12] a discordant datum, in which predicted values are far from observed values and lie outside the general trend of the data set. On the other hand, the least absolute deviations (LAB) method is less sensitive to external errors[13] and is more resistant to outliers than LSQ.[14] LAB gives equal emphasis to all observations, in contrast to LSQ, which gives more weight to large residuals by squaring them. By minimizing sums of absolute values of the residuals rather than the sums of square, the effect of outliers on the coefficient estimate diminishes in the LAB approach. Despite its intrinsic strength, the LAB approach has been under the shadow of LSQ for centuries, even though LAB precedes LSQ by half a century.[15] Boscovich first introduced LAB in his work on the shape of Earth in 1757,[16] and Laplace applied the method to astronomy in 1793.[17] LSQ regression was not developed until later in the early 19th century by Legendre, who predicted the orbits of comets in 1805,[18] and by Gauss, who published the methods in 1809.[19] Moreover, LAB[20−25] is much more needed in the social sciences and economics in particular,[24] where heavy scattering in the data is much more common, due to hidden or unknown variables, than in the natural sciences, in which controlled experiments are more easily performed, with most, if not all, of variables well-defined.

For a common linear system with two parameters, the functions that need to be minimized in each method are the sum of the absolute deviations (SAB) for LAB and the sum of the squares of the deviations (SSQ) for LSQ:

$$\mathrm{SAB} = \sum |Y_i - (b + mX_i)| \quad (1)$$

$$\mathrm{SSQ} = \sum (Y_i - (b + mX_i))^2 \quad (2)$$

where m is the slope and b is the y-intercept.

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Table 1. Comparisons of Results from LSQ, LAB, and MED Methods

Methods	Procedure	Slope ± SD ($m \pm s_m$)	Intercept ± SD ($b \pm s_b$)	SSQ Minimized	SAB Minimized	% SAB
(A) Data from Beer's Law Lab - Actual Student's Data						
LSQ	Excel	4.027 ± 0.099	0.008 ± 0.011	0.001154	0.0748	3.46
	Excel	4.08 ± 0.07	Fixed at 0	0.00131	0.0710	3.28
	Visual	4.03 ± 0.10	0.008 ± 0.01	0.001154	0.0748	3.46
LAB	Solver	4.133 ± 0.112	0.000 ± 0.013	0.00148	0.0673	3.11
	Visual	4.12 ± 0.11	0.00 ± 0.01	0.00147	0.0673	3.11
MED	Theil	4.040 ± 0.10	0.007 ± 0.011	0.001158	0.0750	3.42
	Siegel	4.159 ± 0.12	−0.002 ± 0.01	0.001689	0.0730	3.38
(B) Synthetic Data for Beer's Law for Pronounced Scattering						
Methods	Procedure	Slope ± SD ($m \pm s_m$)	Intercept ± SD ($b \pm s_b$)	SSQ Minimized	SAB Minimized	% SAB
LSQ	Excel	0.6259 ± 0.0563	0.0005 ± 0.0253	0.00601	0.152	11.5
	Visual	0.626 ± 0.078	0.001 ± 0.039	0.00601	0.152	11.5
LAB	Solver	0.5988 ± 0.0601	0.0008 ± 0.0270	0.00694	0.137	10.5
	Visual	0.599 ± 0.060	0.000 ± 0.027	0.00694	0.137	10.5
MED	Theil	0.6043 0.0587	−0.0021 ± 0.0264	0.00685	0.139	10.6
	Siegel	0.6015 ± 0.0602	−0.0013 ± 0.0290	0.00686	0.138	10.6
(C) Data from Massart et al.[36] with an Outlier						
Methods	Procedure	Slope ± SD ($m \pm s_m$)	Intercept ± SD ($b \pm s_b$)	SSQ Minimized	SAB Minimized	% SAB
LSQ	Excel	1.691 ± 0.423	−0.895 ± 1.281	12.5	7.27	36.4
	Visual	1.70 ± 0.42	−0.92 ± 1.28	12.5	7.50	37.5
w/o outlier	Excel	0.960 ± 0.004	0.080 ± 0.094	0.04	0.4	4.0
LAB	Solver	1.032 ± 0.580	0.000 ± 1.756	23.4	5.31	26.6
	Visual	1.03 ± 0.58	0.00 ± 1.76	23.5	5.31	26.6
MED	Theil	1.033 ± 0.58	0.001 ± 1.76	23.4	5.31	26.6
	Siegel	1.017 ± 0.58	0.025 ± 1.77	23.8	5.34	26.7

The difficulties associated with handling the absolute function, which is not differentiable, hindered the development of LAB in its earlier days. Namely, the absolute function in eq 1 is discontinuous, and its derivative is not defined analytically in a single closed form, whereas the function in eq 2 for LSQ is continuous with a well-defined derivative. It is the first derivative that must be set to zero in solving problems of minimization of eqs 1 and 2. This gave the LSQ approach a critical and decisive advantage, leading to its earlier and rapid development in the 19th century and resulting in its current overwhelming dominance over LAB, contributing to its popularity, which appears to be excessive compared with the use of LAB.

Nevertheless, the situation is different nowadays. Namely, new advances in computational technology and statistics since the late 20th century have paved the way for the gradual development of new methods that can minimize the least absolute function numerically.[21−26] These new various numerical approaches utilize iterative algorithms for minimizing LAB and are, in general, more involved and computationally demanding than the ordinary LSQ approach. However, with the development of more efficient optimization programs[25] in recent years, LAB has begun to emerge as a practical tool. LAB minimization is now possible with numerical solver programs, and some are packaged in spreadsheet software, such as the numerical Solver in Excel[7,26,27] that is available as an Add-In. The numerical Solver in Excel,[7,27] in particular, uses algorithms based on the simplex (for linear system) and generalized reduced gradient (for nonlinear system) methods[26] for optimization. Add-Ins of Excel become increasingly popular tools for data analysis, thus being utilized effectively in many places including some laboratory textbooks.[28] In this report, we present results from visual LAB alongside those from numerical LAB using Excel Solver, namely, presenting results from both low (i.e., visual) and high (i.e., using Solver) ends of the numerical approaches.

Both LSQ and LAB methods belong to *M* (maximum likelihood) statistical estimators,[12] which rely on minimization of deviations and are not robust, although LAB is more resistant than LSQ.[12] Thus, it is not surprising to observe the advent of *robust* methods, which are not numerical or noniterative approaches, making them computationally less expensive. These are *L* statistical estimators, which are based on linear combinations of some form of order statistics, such as the median.[12,29] Theil explored such a median (MED) approach[29] using the median values, in which slopes were collected between all possible pairs of points to find the median of all of the $n(n-1)/2$ slopes:[29,30]

$$m_{ij} = (y_j - y_i)/(x_j - x_i) \quad \text{where} \quad x_i \neq x_j,\ 1 \leq i < j \leq n \tag{3}$$

Then the median slope is

$$m_{\mathrm{T}} = \mathrm{med}\{m_{ij}\} \tag{4}$$

The median intercept is found from the median of intercepts found from the median slopes

$$b_{\mathrm{T}} = \mathrm{med}\{y_i - m_{\mathrm{T}}x_i\} \tag{5}$$

Robustness can be given in terms of *breakdown bound* (%), which is the maximum number (in %) of data that can be replaced by arbitrary data with the fit parameters unaffected. While the *M* estimators (LSQ and LAB) have a 0% breakdown bound, Theil's *L* estimator has a value of 29%.[12]

In order to enhance robustness further, the median values were treated further by Siegel;[31] namely, the median of all

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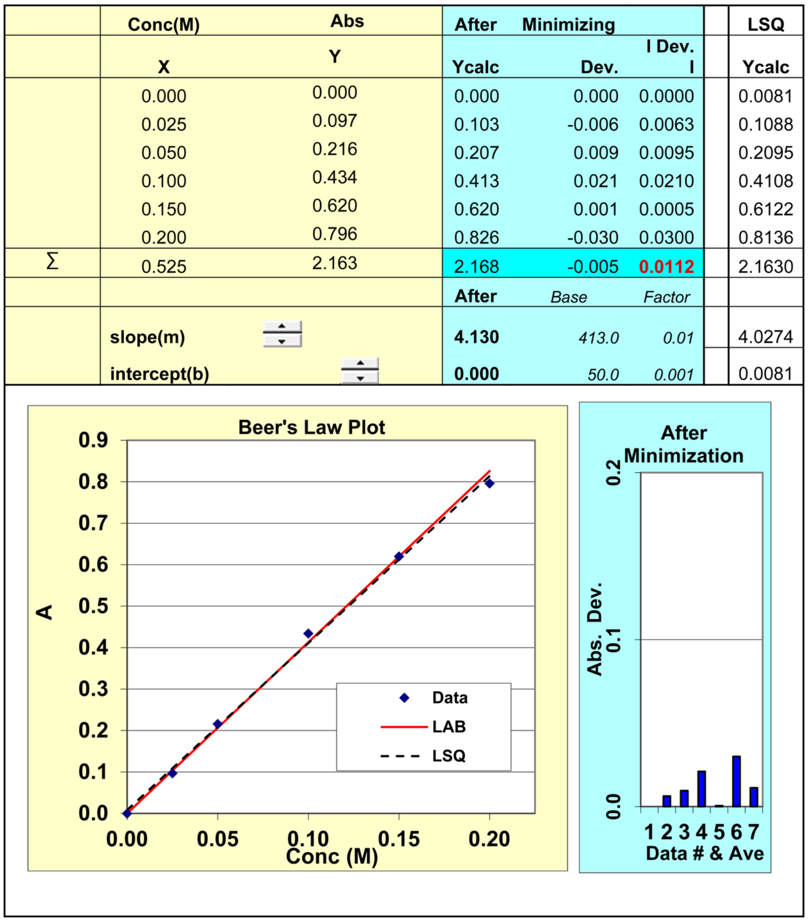

Figure 1. Beer's Law plots with less scattering: minimizing average of abs. dev. Click on the Spinner Buttons to lower the average of the absolute deviations.

slopes for a given point is taken, and the median of these medians is taken as the slope;

$$m_s = \text{med}\{\text{med}\{w_k\}\} \quad (6)$$

where, w_k is the median of all the slopes from a point k.

Then, a new intercept is found with this m_s in similar fashion as Theil,

$$b_s = \text{med}\{y_i - m_s x_i\} \quad (7)$$

The details of algorithm for evaluating m_s and b_s is given in ref 12.

This Siegel's procedure of the repeated median method has a 50% breakdown bound, making it the most robust. Although LAB (visual or numerical) is not as robust as MED, it is resistant to outliers like MED, as shown in the Results section.

In this report, we take both approaches of LAB, that is, visual and numerical (using an algorithm with Excel Solver); at the same time, we also calculated the two parameters of slope (m) and intercept (b) using the MED methods (both Theil's and Siegel's), utilizing the spreadsheet template of Glasser,[12] in order to check how well the four different methods agree. We have already presented this type of visual approach in this journal and others[10] based on the minimization of the least-squares sum, and the visual part of the present work is an extension and sequel of the previous work.[10] This visual approach, based on iterations of trial-and-error, may be referred to as an old-fashioned, yet computer-aided, curve-fitting, or *scientific* "eye-balling", due to the visible displays of the sum of the deviations, absolute or squared, in a bar graph. Interested readers may refer to the Online Supporting Information[10] for detailed examples of visual LSQ in Excel and the supporting documents associated with it; the work is largely based on the interactive spreadsheet approach of Coleman.[32]

■ CALCULATIONS OF STANDARD DEVIATIONS IN THE SLOPE AND INTERCEPT

The standard deviations associated with the two parameters (s_m and s_b) of slope (m) and intercept (b) are calculated from the general formulas for standard deviation based on the variance of the fit (s_y^2). These formulas and examples can be found in several references,[5b,33,34] and the formulas are represented here for clarity:

$$s_y^{\,2} = \frac{\sum (y_i - (b + mx_i))^2}{(N - 2)} \quad (8)$$

$$s_b^{\,2} = \frac{s_y^{\,2} \sum x_i^2}{N \sum x_i^2 - (\sum x_i)^2} \quad (9)$$

$$s_m^{\,2} = \frac{N s_y^{\,2}}{N \sum x_i^2 - (\sum x_i)^2} \quad (10)$$

All of the values of the parameters found by the methods of LSQ, LAB, and MED and the standard deviations associated are summarized in Table 1.

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	X	Y	After Ycal	Minimizing Dev.	I Dev.I	LSQ Ycalc
	0.000	0.000	-0.001	0.001	0.0010	0.0005
	0.100	0.056	0.059	-0.003	0.0029	0.06308
	0.200	0.147	0.119	0.028	0.0282	0.12566
	0.400	0.205	0.239	-0.034	0.0336	0.25082
	0.600	0.430	0.358	0.072	0.0716	0.37598
	0.800	0.479	0.478	0.001	0.0008	0.50114
Σ	2.100	1.317	1.252	0.065	0.0230	1.31718
			After	Base	Factor	
	slope		0.599	599.0	0.001	0.6258
	Intcpt		-0.001	49.0	0.001	0.0005

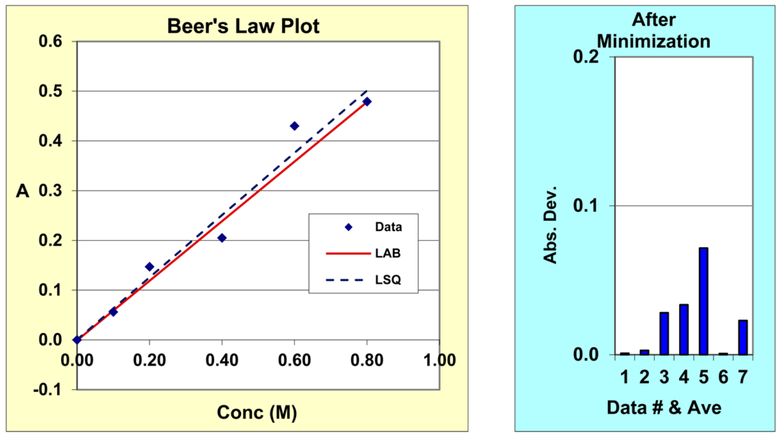

Figure 2. Beer's Law plots with larger scattering: minimizing average of abs. dev. Click on the Spinner Buttons to lower the average of the absolute deviations.

PROCEDURES OF THE VISUAL LEAST ABSOLUTES METHOD (VLAB)

The VLAB is analogous to its visual least squares method (VLSQ) counterpart.[10] The values for the least-squares and related quantities were replaced with those from the least absolutes counterparts. *Please refer to the Excel Template attached in an Appendix*.

Step I. Prepare a table of $X-Y$ data in an Excel worksheet and prepare another column to generate theoretical Y values (Y_{calc}) with any reasonable arbitrary values for slope (m) and intercept (b), which are estimated to start with.

Step II. Calculate the absolute deviations and their average in an additional column. Plot the experimental Y and theoretical Y values in an Excel graph (chart).

Step III. Prepare another graph in a separate chart to represent each of the absolute deviations and their sum or average (the last bar) in a bar graph form.

Step IV. Prepare two spinner bars in order to manipulate the slope and intercept for Y_{calc}. Click on the spinner bar for slope (or intercept) until the height representing the average of the absolute deviations no longer decreases. The first spinner button is to control the slope (m), and the second spinner button is to control the y-intercept (b). Then switch to the other spinner bar to control the intercept (or the slope) and to lower the last bar again. One may alternate back and forth between the slope spinner and intercept spinner bars and repeat the steps until the average is minimized. Lowering of the average bar is easily visible in the beginning, but is often barely recognizable near the end of the process. At this stage, the *y*-scale in the bar graph may be adjusted for an expansion to make it more visible, or the numerical display of the average can be used to see the changes.

DATA AND RESULTS

Beer's Law Experiment with Less Deviations (<5%)

The calculations, graphs, and results are presented in Figure 1 using data from a Beer's Law laboratory. The experiment was taken from "Absorption Spectroscopy and Beer's Law".[35] Students prepared a set of standard solutions (red) of $Co(NO_3)_2{\cdot}6H_2O$ at various concentrations and measured the absorbance of these solutions at 510 nm with a Spectronic 21 (Milton Roy Co.) instrument. Because this is a simple and well-defined system, most students obtain good linear plots with minimal scattering in the data, with a correlation coefficient typically greater than 0.99. The data presented in Figure 1 are actual typical data from a student in a freshman laboratory course (CHEM 1211 Lab) in recent years at Georgia Perimeter College.

The first two columns at the top of the figure are for the original $X-Y$ data. The next three columns are to calculate Y values, deviations, and absolute deviations with any arbitrary values of m and b: only the final results of the minimization are displayed. The last bar in the bar graph represents the average of the absolute deviations (=SAB/6): its numeric value is also displayed in a cell for clarity. This numeric display is helpful when the change in the bar height becomes too small to be visually recognized, particularly near the end of the minimization. The slope and intercept are incremented or decremented by 0.001 and 0.001 (or comparable values) respectively. Since the spinner control for a cell value requires

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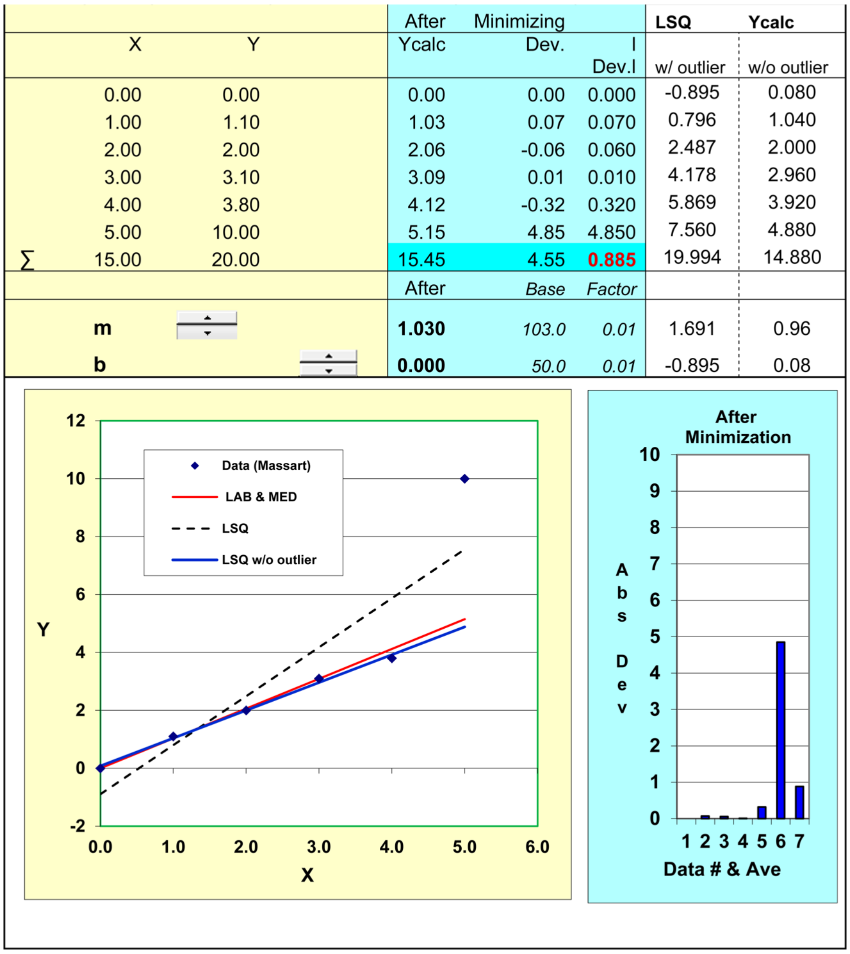

Figure 3. Minimizing average of absolute deviations for a data set with an outlier. Click on Spinners to minimize the average deviation, the last bar in the graph.

an integer increment, the base value is scaled with scaling factors of 0.01 and 0.001 for a fractional increment. For example,

$$\begin{aligned} m &= (\text{the base value}) \times (\text{the scaling factor}) \\ &= 387 \times 0.01 \\ &= 3.87 \end{aligned} \tag{11}$$

$$\begin{aligned} b &= (\text{the base value} - 50) \times (\text{the scaling factor}) \\ &= (57 - 50) \times 0.001 \\ &= 0.007 \end{aligned} \tag{12}$$

For the intercept, however, 50 must be subtracted from the base value in order to allow negative values for this parameter. When the minimization was finally accomplished, it yielded a slope of 4.13 and an intercept of 0.001 with an average deviation of 0.0112 (in a cell of column 6 and row 9) in Figure 1, values that are identical to those obtained with numerical LAB with Solver.

These results are compared with those using LSQ (both from the analytical formula and visual regression) and the MED methods of Theil and Siegel and are summarized in Table 1A for an easy comparison. Columns for SSQ, SAB, and % SAB (= SAB/$\sum Y_i \times 100$) are also given as a criterion for a fit. All six methods yielded similar values with an average slope of 4.08 and an intercept very close to zero. It should noted that the present LAB methods yielded the lowest SAB of 0.06725 and 3.11% SAB, and it agrees well with the results from the Siegel MED method, which yielded the highest slope of 4.159. The LSQ slope (4.03) is closer to Theil's MED slope (4.04), while the LAB slope (4.13) is closer to Siegel's MED slope (4.16). The LAB slope has 0.73% (=(4.13 − 4.10)/4.13 × 100) difference from the average of the two MED slopes, 4.10 (=(4.040 + 4.159)/2), while LSQ slope (=4.03) shows 2.4% difference from the MED slope, which is about 3 times larger than that of LAB: in this respect, LAB slopes agree better with MED slopes than LSQ slopes do. It should be noted that the values of the final (minimized) SSQ and SAB remain nearly the same for all six methods, except the two LAB, which yielded the larger SSQ and smallest SAB and % SAB. All six intercepts are very close to zero, according to Beer's Law. Uncertainties, the two standard deviations (s_m and s_b) associated with the two parameters, are nearly the same: approximately 0.1 for the slope and 0.01 for the intercept.

Beer's Law Data with Larger Scattering with Synthesized Data

We tested the method for a system with heavy scattering in the data in order to demonstrate the effects of exaggerating the deviations with artificial data for the Beer's Law type plot (Figure 2). Namely, the average deviation was made to be larger than 10% of the sum of the y_i values; it was less than 5% in the previous case (Figure 1). The final results are

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summarized in Table 1B for all six methods. The LSQs, whether analytical or visual, yielded nearly the same results, with a slope of 0.626, while LAB and MED yielded nearly identical results of the slope in particular, 0.599 and 0.603 respectively. The LAB slope (=0.599) has about 0.66% difference from the average of the two MED slopes, 0.603 (=(0.6042 + 0.6015)/2), while LSQ slope (=0.626) shows 3.8% difference from the MED slope, which is about 6 times larger than 0.66%: this demonstrate s that LAB slopes agree better with MED slopes than LSQ slopes do. The intercepts are close to zero for all six approaches. It should be noted that LAB and MED yielded a much higher value of SSQ, 0.0069, which is about 12% greater than that of LSQ. However, LAB and MED yielded a much lower value for SAB (ca. 0.138), while LSQ yielded a value of 0.151, which is 10% higher. Basically LAB agrees well with both MED methods; in terms of % SAB, both LAB yielded a result of 10.5%, while both MED methods yielded a result of 10.6%. As far as the uncertainties are concerned, all six methods yielded approximately same values, namely about 0.06 for s_m and about 0.03 for s_b.

A Case with an Outlier for Which LAB Is More Reliable

As the final and most noted case with an outlier, we tested LAB with data that contains an outlier from Massart,[36] which has been well analyzed with the MED methods by Glasser.[12] The visual work is given in Figure 3, and the results are summarized in Table 1 along with others.

The visual LSQ method yielded very similar results to those from the analytical LSQ with a slope of 1.7 and intercept of −0.9. These two values from LSQ are, however, very different from the slopes from LAB and MED; the LAB slope (=1.031) has only 0.59% difference from the average of the two MED slopes, 1.025 (=(1.033 + 1.017)/2), while the LSQ slope (=1.69) shows about 65% difference from the MED slope. The intercepts from both LAB and MED are very close to zero (an average of 0.02), which is again very different than that of LSQs (−0.9). SAB in LAB/MED improved to 5.31 from 7.4 (an average for LSQ). Improvement in % SAB is about 10%, from 38% (LSQ) to 27% (LAB). Because of the outstanding outlier (the last point), the standard deviations of the parameters became very large regardless of the methods employed. LAB/MED, however, yielded larger errors than LSQ, namely, about 30% larger in s_m and 40% larger in s_b.

It is interesting to note that the results of LSQ are closer to the results from LAB/MED with the outlier excluded (5th row from the bottom of the Table) than those with the outlier (7th or 6th row from the bottom). Thus, in this case, one may comfortably discard the outlier, if LSQ must be used, because errors in the parameters were greatly reduced; for the slope in particular, a relative difference from the MED slope became about 6% (=(1.026−0.960)/1.025 × 100) from the previous value of 65%. However, in real situations it is difficult to spot or ignore an outlier regardless of the scattering level; therefore LAB is preferable to LSQ in such a case. It is worth noting that the intercept can be altered without altering the least absolutes sum (SAB), because the standard deviation of the intercept is so large (1.76), deviating greatly from zero.

In general, regardless of the scattering level, whether it is case A (lower scatter) or B (higher scatter), LAB slopes agree with MED slopes within 1%, while LSQ slope agrees within 2−4% depending upon the average deviations. This work proves that the LAB and MED methods yield nearly the same results agreeing well with each other, and this implies that the MED methods of Theil and Siegel are a way to result in a minimization of the SAB, not SSQ, after all.

■ IMPLEMENTATION OF THE VISUAL LAB METHOD IN LABORATORY COURSES

The visual LAB will be helpful in any college courses, including chemistry and physics, where analysis of experimental data requires regression or curve-fitting. Laboratory curricula of general, analytical, or physical chemistry include many such experiments as the common spectrophotometric experiment (Beer's Law lab). The analytical formula and the derivations for the slope (m) and y-intercept (b) from LSQ are commonly treated as a black box without being disclosed to beginning students at lower-level courses; thus the laboratory work and the method could fade away without much retention. In the visual method, however, students actually, see and feel the process of minimizing, and the impression will be better retained, particularly for the visual learners.[37] The Procedure (previous section) can be included in a lab manual for students to follow through it step-by-step working it out by themselves, or an Excel template (of Figure 1) can be distributed to students who are less familiar with the Excel. An Excel Template is appended for the purpose.

■ CONCLUSION

Agreement between the interactive visual and numeric least absolutes method (LAB) is excellent, producing nearly the same results as the median methods (MED) of Theil and Siegel, and is just as easy to implement in the spreadsheet of Excel as is LSQ. As a pedagogical tool, visual LAB is as effective as LSQ since it allows students to actually view the process of regression in terms of minimizing the sum of the absolute deviations in fitting an equation to the data. In the past, we, as educators, scientists, and engineers, have depended mostly on the least-squares method. The time has come to open the door for the Least Absolutes Method, which can handle a system with suspected outliers in a more solid fashion.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.6b00079.

Excel Template for the VLAB (XLSX)

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Notes

The authors declare no competing financial interest.

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